Russell J Boyd

List of Publications by Citations

313 papers	8,294 citations	46 h-index	72 g-index
325 ext. papers	8,647 ext. citations	4.5 avg, IF	5.96 L-index

#	Paper	IF	Citations
313	Electron affinities and ionization potentials of nucleotide bases. *Chemical Physics Letters*, **2000**, 322, 129-135	2.5	213
312	On the importance of prereactive complexes in molecule-radical reactions: hydrogen abstraction from aldehydes by OH. *Journal of the American Chemical Society*, **2001**, 123, 2018-24	16.4	211
311	Extended weak bonding interactions in DNA: pi-stacking (base-base), base-backbone, and backbone-backbone interactions. *Journal of Physical Chemistry B*, **2006**, 110, 563-78	3.4	199
310	Density Functional Study of the Proline-Catalyzed Direct Aldol Reaction. *Journal of Physical Chemistry A*, **2002**, 106, 5155-5159	2.8	172
309	Sulfur-sulfur bond lengths, or can a bond length be estimated from a single parameter?. *Journal of the American Chemical Society*, **1988**, 110, 7299-7301	16.4	164
308	Polarizable point-charge model for water: Results under normal and extreme conditions. *Journal of Chemical Physics*, **1996**, 105, 4742-4750	3.9	162
307	Characterization of a closed-shell fluorine-fluorine bonding interaction in aromatic compounds on the basis of the electron density. *Journal of Physical Chemistry A*, **2005**, 109, 3669-81	2.8	149
306	Group electronegativities from the bond critical point model. *Journal of the American Chemical Society*, **1992**, 114, 1652-1655	16.4	132
305	The shell structure of atoms and the Laplacian of the charge density. *Journal of Chemical Physics*, **1988**, 88, 4375-4377	3.9	131
304	Hydrogen bonding between nitriles and hydrogen halides and the topological properties of molecular charge distributions. *Chemical Physics Letters*, **1986**, 129, 62-65	2.5	127
303	A Density Functional Study of Methanol Clusters. *Journal of Chemical Theory and Computation*, **2007**, 3, 54-61	6.4	118
302	A bond-length-bond-order relationship for intermolecular interactions based on the topological properties of molecular charge distributions. *Chemical Physics Letters*, **1985**, 120, 80-85	2.5	115
301	A theoretical study of 5-halouracils: electron affinities, ionization potentials and dissociation of the related anions. *Chemical Physics Letters*, **2001**, 343, 151-158	2.5	110
300	Atomic and group electronegativities from the electron-density distributions of molecules. *Journal of the American Chemical Society*, **1988**, 110, 4182-4186	16.4	105
299	The 28-Electron Tetraatomic Molecules: N4, CN2O, BFN2, C2O2, B2F2, CBFO, C2FN, and BNO2. Challenges for Computational and Experimental Chemistry. *The Journal of Physical Chemistry*, **1996**, 100, 5702-5714		96
298	Coming to Grips with NHOIN Bonds. 1. Distance Relationships and Electron Density at the Bond Critical Point. *Journal of Physical Chemistry A*, **2001**, 105, 6552-6566	2.8	95
297	An SCFMOCNDO study of equilibrium geometries, force constants, and bonding energies: CNDO/BW. Part I. Parameterization. *Journal of the Chemical Society Dalton Transactions*, **1972**, 73-77		89

296	An Introduction to the Quantum Theory of Atoms in Molecules1-34		88
295	Coulomb hole in some excited states of helium. *Journal of Physics B: Atomic and Molecular Physics*, **1973**, 6, 782-793		86
294	A quantum mechanical explanation for Hund's multiplicity rule. *Nature*, **1984**, 310, 480-481	50.4	84
293	Coming to Grips with N□□□N Bonds. 2. Homocorrelations between Parameters Deriving from the Electron Density at the Bond Critical Point 1. *Journal of Physical Chemistry A*, **2003**, 107, 272-284	2.8	82
292	A theoretical investigation of the structures and properties of peroxyl radicals. *Journal of the American Chemical Society*, **1990**, 112, 5724-5730	16.4	82
291	Six questions on topology in theoretical chemistry. *Computational and Theoretical Chemistry*, **2015**, 1053, 2-16	2	81
290	Comparison of Experimental and Calculated Hyperfine Coupling Constants. Which Radicals Are Formed in Irradiated Guanine?. *Journal of Physical Chemistry B*, **1998**, 102, 9332-9343	3.4	78
289	Radiation Products of Thymine, 1-Methylthymine, and Uracil Investigated by Density Functional Theory. *Journal of Physical Chemistry B*, **1998**, 102, 5369-5377	3.4	76
288	Tautomeric Equilibria of Hydroxypyridines in Different Solvents: An ab Initio Study. *The Journal of Physical Chemistry*, **1996**, 100, 16141-16146		73
287	Selenium stories. *Nature Chemistry*, **2011**, 3, 570	17.6	72
286	The Fermi hole in atoms. *Journal of Physics B: Atomic and Molecular Physics*, **1974**, 7, 1805-1816		67
285	Theoretical Investigation of Adenine Radicals Generated in Irradiated DNA Components. *Journal of Physical Chemistry B*, **1998**, 102, 10602-10614	3.4	66
284	Molecular model with quantum mechanical bonding information. *Journal of Physical Chemistry A*, **2011**, 115, 12991-7	2.8	63
283	Cooperativity between hydrogen bonds and beryllium bonds in (H2O)(n)BeX2 (n = 1-3, X = H, F) complexes. A new perspective. *Physical Chemistry Chemical Physics*, **2012**, 14, 14540-7	3.6	62
282	Effects of Ionizing Radiation on Crystalline Cytosine Monohydrate. *Journal of Physical Chemistry B*, **1998**, 102, 7484-7491	3.4	62
281	An ab initio study of model SN2 reactions with inclusion of electron correlation effects through second-order Moeller-Plesset perturbation calculations. *Journal of the American Chemical Society*, **1990**, 112, 6789-6796	16.4	61
280	Alkoxy radicals in the gaseous phase: ß-scission reactions and formation by radical addition to carbonyl compounds. *Canadian Journal of Chemistry*, **2003**, 81, 431-442	0.9	55
279	The relative sizes of atoms. *Journal of Physics B: Atomic and Molecular Physics*, **1977**, 10, 2283-2291		55

278	Transition-state electronic structures in SN2 reactions. *Journal of the American Chemical Society*, **1989**, 111, 1575-1579	16.4	53
277	Changing weak halogen bonds into strong ones through cooperativity with beryllium bonds. *Journal of Physical Chemistry A*, **2014**, 118, 4205-13	2.8	51
276	Electron density partitioning in atoms. *Journal of Chemical Physics*, **1977**, 66, 356-358	3.9	50
275	Atomic contributions to bond dissociation energies in aliphatic hydrocarbons. *Journal of Chemical Physics*, **2006**, 125, 204103	3.9	49
274	Ab initio studies of reactions of hydroxyl radicals with fluorinated ethanes. *The Journal of Physical Chemistry*, **1995**, 99, 13402-13411		48
273	A hybrid quantum mechanical force field molecular dynamics simulation of liquid methanol: Vibrational frequency shifts as a probe of the quantum mechanical/molecular mechanical coupling. *Journal of Chemical Physics*, **1996**, 104, 7261-7269	3.9	48
272	Electronic and structural properties of borazine and related molecules. *Chemical Physics Letters*, **1984**, 112, 136-141	2.5	48
271	QTAIM study of an alpha-helix hydrogen bond network. *Journal of Physical Chemistry B*, **2009**, 113, 10957-64	3.4	46
270	Stereoselective synthesis of a potent thrombin inhibitor by a novel P2-P3 lactone ring opening. *Journal of Organic Chemistry*, **2004**, 69, 3620-7	4.2	46
269	Sulfonyl radicals, sulfinic acid, and related species: an abinitio molecular orbital study. *Canadian Journal of Chemistry*, **1980**, 58, 331-338	0.9	46
268	Electronegativities of the elements from a nonempirical electrostatic model. *Journal of Chemical Physics*, **1981**, 75, 5385-5388	3.9	46
267	Density functional theory study of the reaction mechanism and energetics of the reduction of hydrogen peroxide by ebselen, ebselen diselenide, and ebselen selenol. *Journal of Physical Chemistry A*, **2007**, 111, 3152-60	2.8	44
266	A Comprehensive Study of Sugar Radicals in Irradiated DNA. *Journal of Physical Chemistry B*, **1998**, 102, 7674-7686	3.4	44
265	van der Waals Complexes of Water with Oxygen and Nitrogen: Infrared Spectra and Atmospheric Implications. *Journal of Physical Chemistry A*, **1998**, 102, 7294-7296	2.8	44
264	The first example of a cage critical point in a single ring: A novel twisted □-helical ring topology. *Chemical Physics Letters*, **2005**, 409, 265-269	2.5	43
263	Electronic structure calculations of hydrocarbon radical cations: a density functional study. *Journal of the American Chemical Society*, **1993**, 115, 6896-6900	16.4	43
262	The effect of electron correlation on the topological and atomic properties of the electron density distributions of molecules. *Journal of Computational Chemistry*, **1989**, 10, 367-375	3.5	43
261	The shell structure of atoms. *Journal of Physics B: Atomic and Molecular Physics*, **1976**, 9, L69-L72		43

260	Effects of electron correlation on the series C2HnF6-n (n = 0-6): geometries, total energies, and C-C and C-H bond dissociation energies. *The Journal of Physical Chemistry*, **1993**, 97, 7208-7215		41
259	Recent applications of density functional theory calculations to biomolecules. *Theoretical Chemistry Accounts*, **2002**, 108, 1-11	1.9	40
258	A Density-Functional Theory Investigation of the Radiation Products of l-α-Alanine. *Journal of Physical Chemistry A*, **1999**, 103, 4303-4308	2.8	40
257	A comparative study of the hyperfine structures of neutral nitrogen oxides: DFT vs CISD results. *The Journal of Physical Chemistry*, **1994**, 98, 792-799		40
256	Density functional theory investigation of hyperfine coupling constants in peroxyl radicals. *Journal of Chemical Physics*, **1997**, 106, 7738-7748	3.9	39
255	The radial density function for the neutral atoms from helium to xenon. *Canadian Journal of Physics*, **1977**, 55, 452-455	1.1	39
254	A Quantum Chemical and TST Study of the OH Hydrogen-Abstraction Reaction from Substituted Aldehydes: FCHO and ClCHO. *Journal of Physical Chemistry A*, **2001**, 105, 9034-9039	2.8	38
253	Intracule densities and electron correlation in the hydrogen molecule. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **1988**, 21, 2555-2561	1.3	38
252	Diazasilene (SiNN): a comparative study of electron density distributions derived from Hartree-Fock, second-order Moller-Plesset perturbation theory, and density functional methods. *The Journal of Physical Chemistry*, **1994**, 98, 1844-1850		37
251	Fluorine-fluorine spin-spin coupling constants in aromatic compounds: correlations with the delocalization index and with the internuclear separation. *Journal of Chemical Information and Modeling*, **2005**, 45, 354-9	6.1	36
250	The Spin Dependence of the Spatial Size of Fe(II) and of the Structure of Fe(II)-Porphyrins. *Journal of Physical Chemistry A*, **2004**, 108, 4653-4657	2.8	36
249	Effect of substituents on the GPx-like activity of ebselen: steric versus electronic. *Journal of Physical Chemistry A*, **2008**, 112, 1013-7	2.8	35
248	Modeling the reaction mechanisms of the amide hydrolysis in an N-(o-carboxybenzoyl)-L-amino acid. *Journal of the American Chemical Society*, **2003**, 125, 6994-7000	16.4	35
247	Structure sensitivity and cluster size convergence for formate adsorption on copper surfaces: A DFT cluster model study. *Journal of Chemical Physics*, **2000**, 112, 9562-9568	3.9	35
246	A Density Functional Theory Study of the Radiation Products of Glycine. *Journal of Physical Chemistry A*, **2000**, 104, 5080-5086	2.8	35
245	A Theoretical Study of the Effects of Protonation and Deprotonation on Bond Dissociation Energies. *Journal of the American Chemical Society*, **1995**, 117, 8816-8822	16.4	35
244	Theoretical study of metastable N2CO isomers. New candidates for high energy materials?. *Chemical Physics Letters*, **1994**, 227, 312-320	2.5	35
243	A localized electrons detector for atomic and molecular systems. *Theoretical Chemistry Accounts*, **2010**, 127, 393-400	1.9	34

242	Theoretical studies of the cross-linking mechanisms between cytosine and tyrosine. *Journal of the American Chemical Society*, **2002**, 124, 2753-61	16.4	34
241	The Laplacian of the charge density as a probe of reaction paths and reactivity: a comparison of SN2 reactions at carbon and silicon. *The Journal of Physical Chemistry*, **1991**, 95, 4698-4701		34
240	Hydrogen bond cooperativity in water hexamers: atomic energy perspective of local stabilities. *Journal of Physical Chemistry A*, **2013**, 117, 10790-9	2.8	33
239	Electron Densities of Several Small Molecules As Calculated from Density Functional Theory. *The Journal of Physical Chemistry*, **1996**, 100, 6317-6324		33
238	An SCF-MO-CNDO study of equilibrium geometries, force constants, and bonding energies: CNDO/BW. Part II. Diatomics. *Journal of the Chemical Society Dalton Transactions*, **1972**, 78-81		33
237	A density functional theory study of the hyperfine structures of the atoms B to O and the species NH2 and NH+3. *Chemical Physics Letters*, **1994**, 217, 24-30	2.5	32
236	Density difference representation of electron correlation. *Journal of Chemical Physics*, **1978**, 68, 1951-1957	3.9	32
235	Visualizing internal stabilization in weakly bound systems using atomic energies: hydrogen bonding in small water clusters. *Journal of Physical Chemistry A*, **2012**, 116, 3946-51	2.8	31
234	The Hydrated Electron as a Pseudo-Atom in Cavity-Bound Water Clusters. *Journal of Chemical Theory and Computation*, **2007**, 3, 1054-63	6.4	31
233	Topological Atom-Atom Partitioning of Molecular Exchange Energy and its Multipolar Convergence121-140		31
232	Modeling the reduction of hydrogen peroxide by glutathione peroxidase mimics. *Journal of Physical Chemistry A*, **2006**, 110, 8979-85	2.8	31
231	The Radius of the Coulomb Hole. *Canadian Journal of Physics*, **1975**, 53, 592-597	1.1	31
230	Secondary H/D isotope effects and transition state looseness in nonidentity methyl transfer reactions. Implications for the concept of enzymic catalysis via transition state compression. *Journal of the American Chemical Society*, **1993**, 115, 10147-10152	16.4	30
229	A density functional theory study of the free radicals NH2, NF2, NCl2, PH2, PF2, and PCl2. *Canadian Journal of Chemistry*, **1994**, 72, 695-704	0.9	30
228	The effect of electron correlation on the electron density distributions of molecules: Comparison of perturbation and configuration interaction methods. *Journal of Chemical Physics*, **1989**, 90, 1083-1090	3.9	30
227	Energy component analysis of the Jahn-Teller effect in the methane radical cation. *Journal of Chemical Physics*, **1991**, 94, 8083-8088	3.9	30
226	Intrinsic barriers of some model SN2 reactions: second-order Moeller-Plesset perturbation calculations. *Journal of the American Chemical Society*, **1991**, 113, 2434-2439	16.4	30
225	Hund's rule and singlet-triplet energy differences for molecular systems. *Journal of Chemical Physics*, **1987**, 87, 5329-5332	3.9	30

224	A theoretical investigation of the 1,3-migration in allylperoxyl radicals. *Journal of the American Chemical Society*, **1993**, 115, 687-693	16.4	29
223	Can correlation bring electrons closer together?. *Molecular Physics*, **2009**, 107, 1089-1093	1.7	28
222	On the local representation of the electronic momentum operator in atomic systems. *Journal of Chemical Physics*, **2008**, 129, 024110	3.9	28
221	Recombination of methyl radicals: ab initio potential and transition-state theory calculations. *The Journal of Physical Chemistry*, **1989**, 93, 4772-4779		28
220	Interpretation of Hund's rule for first-row hydrides AH (A = lithium, boron, nitrogen, fluorine). *The Journal of Physical Chemistry*, **1990**, 94, 3480-3484		28
219	Charge development at the transition state: a second-order Moeller-Plesset perturbation study of gas-phase SN2 reactions. *Journal of the American Chemical Society*, **1991**, 113, 1072-1076	16.4	28
218	Angular aspects of electron correlation and the Coulomb hole. *Journal of Chemical Physics*, **1982**, 77, 3578-3582	3.9	28
217	The Coulomb hole in the 23S state of the helium isoelectronic sequence. *International Journal of Quantum Chemistry*, **1974**, 8, 255-261	2.1	28
216	Relative sizes of high and low spin states of atoms. *Nature*, **1974**, 250, 566-567	50.4	28
215	An evaluation of various computational methods for the treatment of organoselenium compounds. *Journal of Physical Chemistry A*, **2005**, 109, 10373-9	2.8	27
214	A Computational Study of the Kinetics of the NO3Hydrogen-Abstraction Reaction from a Series of Aldehydes (XCHO:X = F, Cl, H, CH3). *Journal of Physical Chemistry A*, **2002**, 106, 384-394	2.8	27
213	Charge and intracule densities in singly excited heliumlike ions. *Journal of Chemical Physics*, **1993**, 98, 7132-7139	3.9	27
212	A Comparative Study of Electron Densities in Carbon Monoxide Calculated from Conventional ab Initio and Density Functional Methods. *The Journal of Physical Chemistry*, **1994**, 98, 6988-6994		27
211	An ab initio SCF calculation of the effect of water-anion and water-cation interactions on the vibrational frequencies of water. *Spectrochimica Acta Part A: Molecular Spectroscopy*, **1986**, 42, 175-180		27
210	The Ionezation Potentials of BF3, BC13 and BBr3. *Chemical Physics Letters*, **1968**, 1, 649-650	2.5	27
209	The effect of multiplicity on the size of iron(II) and the structure of iron(II) porphyrins. *Journal of Physical Chemistry A*, **2010**, 114, 10315-9	2.8	25
208	Reduction of hydrogen peroxide by glutathione peroxidase mimics: reaction mechanism and energetics. *Journal of Physical Chemistry A*, **2010**, 114, 1996-2000	2.8	25
207	Evaluation of effective core potentials and basis sets for the prediction of the geometries of alkyltin halides. *Journal of Physical Chemistry A*, **2006**, 110, 5893-6	2.8	25

206	An ab initio study of the series of fluorinated ethanes C2HnF6-n (n = 0-6): geometries, total energies, and carbon-carbon bond dissociation energies. *The Journal of Physical Chemistry*, **1992**, 96, 6287-6290		25
205	Hund's rule and singlet–triplet energy differences for the lowest n→π* states of formaldehyde, H2CO. *Journal of Chemical Physics*, **1989**, 90, 5638-5643	3.9	25
204	Thermochemical parameters for organic radicals and radical ions. Part 2. The protonation of hydrocarbon radicals in the gas phase. *Canadian Journal of Chemistry*, **1982**, 60, 3011-3018	0.9	25
203	The effect of electron correlation on one-electron distributions. *Chemical Physics Letters*, **1976**, 44, 363-365	2.3	25
202	Properties of Transition Species in the Reaction of Hydroxyl with Ethane from ab Initio Calculations and Fits to Experimental Data. *The Journal of Physical Chemistry*, **1995**, 99, 8661-8668		24
201	Torquoselectivity in the Nazarov reactions of allenyl vinyl ketones. *Journal of Organic Chemistry*, **2015**, 80, 1042-51	4.2	23
200	Assessment of several DFT functionals in calculation of the reduction potentials for Ni-, Pd-, and Pt-bis-ethylene-1,2-dithiolene and -diselenolene complexes. *Journal of Physical Chemistry A*, **2015**, 119, 911-8	2.8	23
199	A density functional theory study of the dimers of HX (X = F, Cl, and Br). *Journal of Computational Chemistry*, **2001**, 22, 1590-1597	3.5	23
198	A Computational Study of the Isomerization of Prolyl Amides As Catalyzed by Intramolecular Hydrogen Bonding. *Journal of Physical Chemistry A*, **2002**, 106, 11168-11172	2.8	23
197	Modeling the action of an antitumor drug: a density functional theory study of the mechanism of tirapazamine. *Journal of the American Chemical Society*, **2001**, 123, 7320-5	16.4	23
196	Conformations of simple disulfides and L-cystine. *Canadian Journal of Chemistry*, **1983**, 61, 1082-1085	0.9	23
195	1,n-Radical ions: an abinitio study of racemization and isomerization of the cyclopropane radical cation. *Canadian Journal of Chemistry*, **1985**, 63, 3283-3289	0.9	23
194	Systematic study of the performance of density functional theory methods for prediction of energies and geometries of organoselenium compounds. *Journal of Physical Chemistry A*, **2011**, 115, 4827-31	2.8	22
193	A density functional theory study of the mechanism of the Paal–Knorr pyrrole synthesis. *Computational and Theoretical Chemistry*, **2007**, 811, 97-107		22
192	Molecular structures and excited states of CpM(CO)(2) (Cp = eta(5)-C(5)H(5); M = Rh, Ir) and [Cl(2)Rh(CO)(2)](-). Theoretical evidence for a competitive charge transfer mechanism. *Journal of the American Chemical Society*, **2002**, 124, 2664-71	16.4	22
191	An assessment of theoretical methods for the study of transition metal carbonyl complexes: $[Cl_2Rh(CO)_2]^-$ and $[Cl_2Rh(CO)]^-$ as case studies. *Journal of Chemical Physics*, **2000**, 113, 9393-9401	3.9	22
190	Stereoselectivity of nucleophilic addition to substituted cyclohexanones: a structure and charge density study. *Journal of the American Chemical Society*, **1993**, 115, 9614-9619	16.4	22
189	The evaluation of extracule and intracule densities in the first-row hydrides, LiH, BeH, BH, CH, NH, OH and FH, from self-consistent field molecular orbital wavefunctions. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **1990**, 23, 1095-1105	1.3	22

188	Balancing Exchange Mixing in Density-Functional Approximations for Iron Porphyrin. *Journal of Chemical Theory and Computation*, **2015**, 11, 3022-8	6.4	21
187	Statistical electron correlation coefficients for 29 states of the heliumlike ions. *International Journal of Quantum Chemistry*, **1993**, 48, 33-42	2.1	21
186	Angular aspects of exchange correlation and the fermi hole. *International Journal of Quantum Chemistry*, **1985**, 27, 439-449	2.1	21
185	Thermal and photochemical reactivity of cyclopropene derivatives: a semi-empirical molecular orbital study. *Canadian Journal of Chemistry*, **1977**, 55, 2482-2491	0.9	21
184	Theoretical Study of the Effects of Protonation and Deprotonation on Bond Dissociation Energies of Second-Row Elements: Comparison with First-Row Elements. *Journal of the American Chemical Society*, **1997**, 119, 4214-4219	16.4	20
183	Validation of a computational scheme to study 15N and 13C nuclear shielding constants. *Chemical Physics Letters*, **2005**, 401, 7-12	2.5	20
182	Addition vs Abstraction Reactions of the Methyl Radical with Nitrones, Alkenes, Aldehydes, and Imines. *Journal of Physical Chemistry A*, **2001**, 105, 7096-7105	2.8	20
181	Electron Densities of Homonuclear Diatomic Molecules As Calculated from Density Functional Theory. *The Journal of Physical Chemistry*, **1996**, 100, 5274-5280		20
180	The effect of a neon matrix on the hyperfine structure of CH+4. A model study. *Chemical Physics Letters*, **1993**, 211, 88-93	2.5	20
179	Computational Study of Engineered Cytochrome P450-Catalyzed C-H Amination: The Origin of the Regio- and Stereoselectivity. *Journal of Physical Chemistry B*, **2017**, 121, 10859-10868	3.4	19
178	Is the size of an atom determined by its ionization energy?. *Chemical Physics Letters*, **2009**, 480, 127-131	2.5	19
177	Theoretical Studies of the Radiation Products of Hydroxyproline. *Journal of Physical Chemistry A*, **2000**, 104, 8583-8592	2.8	19
176	The lone electron pair and crystal packing: observations on pyramidal YEL3 species, abinitio calculations, and the crystal structures of Me3SOI, Et3SI, (Me3S)2SnCl6, (Me3SO)2SnCl6, and (Et3S)2SnCl6. *Canadian Journal of Chemistry*, **1989**, 67, 1984-2008	0.9	19
175	Photoelectron spectra of diazabasketene, diazadeltacyclene, and related polycyclic cis-azoalkanes. *Journal of the American Chemical Society*, **1976**, 98, 2398-2406	16.4	19
174	Electronic energy changes associated with Guanine quadruplex formation: an investigation at the atomic level. *Journal of Physical Chemistry B*, **2010**, 114, 9833-9	3.4	18
173	Calculation of Quadrupole Moments of Polycyclic Aromatic Hydrocarbons: Applications to Chromatography. *Journal of Physical Chemistry A*, **1997**, 101, 5374-5377	2.8	18
172	Modeling competitive reaction mechanisms of peroxynitrite oxidation of guanine. *Journal of Physical Chemistry A*, **2006**, 110, 9908-14	2.8	18
171	Hyperfine Structures of the Series C2HnF5-n, n = 0-5: A Density Functional Theory Study. *The Journal of Physical Chemistry*, **1995**, 99, 623-629		18

170	Conformational aspects of L-histidine. *Canadian Journal of Chemistry*, **1981**, 59, 3232-3236	0.9	18
169	AB initio calculations of 2H and 14N quadrupolar coupling constants in hydrogen bonded dimers. *Chemical Physics Letters*, **1982**, 89, 478-482	2.5	18
168	Photoelectron spectra of 2,3-diazabicyclo[2.2.n]alk-2-enes (n = 1,2,3,4). *Journal of the American Chemical Society*, **1973**, 95, 6478-6480	16.4	18
167	Bond length and the electron density at the bond critical point: X--X, Z--Z, and C--Z bonds (X = Li-F, Z = Na-Cl). *Journal of Computational Chemistry*, **2008**, 29, 367-79	3.5	17
166	Efficient synthesis of the optically active dihydropyrimidinone of a potent □1A- selective adrenoceptor antagonist. *Canadian Journal of Chemistry*, **2002**, 80, 646-652	0.9	17
165	A theoretical study of the change in homolytic bond dissociation energy on conversion of A-B to A-B+H. *Journal of the American Chemical Society*, **1989**, 111, 5152-5155	16.4	17
164	On the relationship between the electron-pair distribution function and the correlation energy of an atom. *International Journal of Quantum Chemistry*, **1986**, 29, 1-9	2.1	17
163	Atomic orbital populations and atomic charges from self-consistent field molecular orbital wavefunctions. *Journal of the Chemical Society, Faraday Transactions 2*, **1987**, 83, 1307		17
162	1,n-Radical ions: the nature of the one-electron two-centre bond in cyclopropane radical cations. An abinitio SCF MO approach. *Canadian Journal of Chemistry*, **1983**, 61, 2310-2315	0.9	17
161	cis-Azoxyalkanes. III. Dichotomy in the thermal stability of azo- and azoxyalkanes. *Journal of the American Chemical Society*, **1972**, 94, 3260-3261	16.4	17
160	Atomic energy analysis of cooperativity, anti-cooperativity, and non-cooperativity in small clusters of methanol, water, and formaldehyde. *Computational and Theoretical Chemistry*, **2015**, 1053, 328-336	2	16
159	Kinetics and Thermodynamics of the Monomer□Dimer Equilibria of Dialkoxydibutylstannanes. *Organometallics*, **2010**, 29, 6384-6392	3.8	16
158	Electronegativity and Hardness of Disjoint and Transferable Molecular Fragments. *The Journal of Physical Chemistry*, **1996**, 100, 3448-3453		16
157	Modeling the reaction mechanisms of the imide formation in an N-(o-carboxybenzoyl)-L-amino acid. *Journal of the American Chemical Society*, **2003**, 125, 3642-8	16.4	16
156	A combined quantum mechanics and molecular dynamics study of small Jahn□Teller distorted hydrocarbons: Another difficult test for density-functional theory. *Journal of Chemical Physics*, **1999**, 110, 12059-12069	3.9	16
155	On the systematic behaviour of certain Hartree-Fock expectation values. *Journal of Physics B: Atomic and Molecular Physics*, **1978**, 11, L655-L658		16
154	A theoretical study of proton transfers in aqueous para-, ortho-hydroxypyridine and para-, ortho-hydroxyquinoline. *Chemical Physics Letters*, **1996**, 259, 647-653	2.5	15
153	The interactions between alkali metals and C2H2. Density functional theory as an analytic tool. *Chemical Physics Letters*, **1995**, 235, 422-429	2.5	15

152	The first-order Jahn□eller distortion and the symmetry of the electron density in the BH+3 radical. *Journal of Chemical Physics*, **1992**, 96, 1232-1239	3.9	15
151	Fermi and Coulomb correlations in the 21 S state of the helium isoelectronic sequence. *Theoretica Chimica Acta*, **1977**, 45, 61-67		15
150	Orbital energie and charge densities in borazine. *Chemical Physics Letters*, **1968**, 2, 227-229	2.5	15
149	Theoretical investigations on the reaction of monosubstituted tertiary-benzylamine selenols with hydrogen peroxide. *Journal of Physical Chemistry A*, **2010**, 114, 10706-11	2.8	14
148	Density functional theory studies of the quadrupole moments of benzene and naphthalene. *Chemical Physics Letters*, **1997**, 277, 252-256	2.5	14
147	Gas-Phase Interaction of Calcium (Ca(2+)) with Seleno Derivatives of Uracil. *Journal of Chemical Theory and Computation*, **2008**, 4, 1002-11	6.4	14
146	The topological features of the intracule density of the uniform electron gas. *Chemical Physics Letters*, **1999**, 304, 393-398	2.5	14
145	Molecular orbital treatment of substituent effects. I. Structures of some carbon acids and their conjugate bases. *Canadian Journal of Chemistry*, **1983**, 61, 45-49	0.9	14
144	An SCF□MO□CNDO study of equilibrium geometries, force constants, and bonding energies: CNDO/BW. Part III. Triatomics and polyatomics. *Journal of the Chemical Society Dalton Transactions*, **1972**, 81-87		14
143	Mechanism of the Reduction of an Oxidized Glutathione Peroxidase Mimic with Thiols. *Journal of Chemical Theory and Computation*, **2012**, 8, 5052-7	6.4	13
142	Revealing unexpected mechanisms for nucleophilic attack on S-S and Se-Se bridges. *Chemistry - A European Journal*, **2013**, 19, 3629-38	4.8	13
141	Crystal chemistry of tetraradial species. Part 10. Tilting at windmills: conformations of the tetraphenyl species ZPh40, □1 (Z = B, C, N). *Canadian Journal of Chemistry*, **2002**, 80, 1351-1366	0.9	13
140	The 2□ states of HBeO, HMgO, and HCaO. *Journal of Chemical Physics*, **1996**, 104, 4055-4060	3.9	13
139	A Theoretical Study of Spin Trapping by Nitrone: Trapping of Hydrogen, Methyl, Hydroxyl, and Peroxyl Radicals. *The Journal of Physical Chemistry*, **1994**, 98, 11705-11713		13
138	Cleavage of the radical cations of alkenes; 1-butene and 4,4-dimethyl-1-pentene. Ab initio calculations on the interaction between the allyl and alkyl radical and carbocation moieties. *Canadian Journal of Chemistry*, **1991**, 69, 1365-1375	0.9	13
137	Ab-initio molecular orbital study of the cis/trans conformations of the peptide bond. *International Journal of Quantum Chemistry*, **1981**, 20, 117-127	2.1	13
136	Intracule and Extracule Densities: Historical Perspectives and Future Prospects. *Mathematical and Computational Chemistry*, **2000**, 231-248		13
135	Bond critical points in the electronic structures of the main group diatomic hydrides of lithium through bromine. *Journal of Computational Chemistry*, **1987**, 8, 489-498	3.5	12

134	On the Fermi hole in atoms. *Journal of Physics B: Atomic and Molecular Physics*, **1975**, 8, L130-L133		12
133	The radial density function and expectation values for ions. *Canadian Journal of Physics*, **1978**, 56, 780-780	1.1	12
132	An SCF MO CNDO study of ionization potentials and orbital energies by the CNDO/BW theory. *The Journal of the Chemical Society A, Inorganic, Physicaloretical*, **1971**, 3579-3589		12
131	The one-electron reduction of dithiolate and diselenolate ligands. *Physical Chemistry Chemical Physics*, **2014**, 16, 10897-902	3.6	11
130	QTAIM in Drug Discovery and Protein Modeling471-498		11
129	Angular aspects of electron correlation and the Coulomb hole. II. The 2 1S and the 2 3S excited states of helium. *Journal of Chemical Physics*, **1987**, 87, 1216-1219	3.9	11
128	An Electron Density Source-Function Study of DNA Base Pairs in Their Neutral and Ionized Ground States. *Journal of Computational Chemistry*, **2018**, 39, 1112-1128	3.5	10
127	Organotin bond dissociation energies: An interesting challenge for contemporary computational methods. *Computational and Theoretical Chemistry*, **2014**, 1050, 7-14	2	10
126	Factors controlling extremely strong AAA-DDD triply hydrogen-bonded complexes. *Chemical Physics Letters*, **2008**, 450, 210-213	2.5	10
125	The effect of electron-withdrawing groups on 15N and 13C chemical shifts: a density functional study on a series of pyrroles. *Molecular Physics*, **2005**, 103, 1113-1129	1.7	10
124	Effects of Alkyl Substituents on the Excited States of Naphthalene: Semiempirical Study. *Journal of Physical Chemistry A*, **2000**, 104, 1020-1029	2.8	10
123	Ab Initio Studies of the Contrasting Butadiene Cheletropic and Diels Alder Cycloaddition Reactivities Observed for Carbenic Phosphorus (Phosphenium) and Arsenic (Arsenium) Cations *Organometallics*, **1998**, 17, 4014-4029	3.8	10
122	Protonation and Deprotonation Effects on the Chemistry of the Third-Row Elements: Homolytic versus Heterolytic Cleavage. *Journal of Physical Chemistry A*, **1999**, 103, 7087-7093	2.8	10
121	CaOH has a second linear structure HCaO. *Journal of Chemical Physics*, **1995**, 103, 10070-10073	3.9	10
120	Internal motion of benzene. A molecular dynamics simulation study. *Chemical Physics Letters*, **1995**, 241, 380-386	2.5	10
119	Singlet-triplet energy component differences in homonuclear diatomics: A multi-reference configuration interaction study of Hund's rule. *Chemical Physics*, **1991**, 157, 99-104	2.3	10
118	Electron correlation effects in the Rydberg-like 33D and 31D states of helium-like ions. *International Journal of Quantum Chemistry*, **1993**, 48, 1-14	2.1	10
117	Geometries, energies and polarities of cyanopolyynes. *Chemical Physics*, **1981**, 58, 203-210	2.3	10

116	Refinement of the SAVE SCF MO CNDO theory. Part I. Bonding parameters. *The Journal of the Chemical Society A, Inorganic, Physicaloretical*, **1969**, 2598-2600		10
115	On the Bond Order between Atoms in Approximate SCF-MO Theory. *Canadian Journal of Chemistry*, **1973**, 51, 1151-1154	0.9	10
114	Scaling in the S and P states of the helium isoelectronic sequence. *Theoretica Chimica Acta*, **1974**, 33, 79-86		10
113	Identifying similarities and differences between analogous bisdithiolene and bisdiselenolene complexes: A computational study. *International Journal of Quantum Chemistry*, **2016**, 116, 369-376	2.1	9
112	Effect of amino acid ligands on the structure of iron porphyrins and their ability to bind oxygen. *Journal of Physical Chemistry A*, **2014**, 118, 4565-74	2.8	9
111	Effect of Sr2+ association on the tautomerization processes of uracil and its dithio- and diseleno-derivatives. *Organic and Biomolecular Chemistry*, **2011**, 9, 423-31	3.9	9
110	Theoretical study of polaron formation in poly(G)-poly(C) cations. *Journal of Physical Chemistry B*, **2011**, 115, 3136-45	3.4	9
109	Interpretation of Experimental Electron Densities by Combination of the QTAMC and DFT257-283		9
108	Topological Properties of the Electron Distribution in Hydrogen-bonded Systems425-451		9
107	Calibration of a computational scheme for solvation: Group I and II metal ions bound to water, formaldehyde and ammonia. *Molecular Physics*, **2005**, 103, 337-344	1.7	9
106	The calculation of accurate 17O hyperfine coupling constants in the hydroxyl radical: A difficult problem for current quantum chemical methods. *Journal of Chemical Physics*, **1998**, 109, 9451-9462	3.9	9
105	Reply to Comment on Effects of Ionizing Radiation on Crystalline Cytosine Monohydrate *Journal of Physical Chemistry B*, **1999**, 103, 3051-3052	3.4	9
104	Effect of an adding radical's electronegativity on the geometries and formation energies of nitroso spin adducts. *The Journal of Physical Chemistry*, **1994**, 98, 1856-1863		9
103	Molecular orbital treatment of substituent effects. II. Structures of some carboxylic Acids and their conjugate bases. *Canadian Journal of Chemistry*, **1984**, 62, 2881-2886	0.9	9
102	Molecular orbital treatment of substituent effects. III. Proton affinities of some methyl and carboxylate anions. *Canadian Journal of Chemistry*, **1984**, 62, 2887-2891	0.9	9
101	Computational Examination of (4 + 3) versus (3 + 2) Cycloaddition in the Interception of Nazarov Reactions of Allenyl Vinyl Ketones by Dienes. *Journal of Organic Chemistry*, **2015**, 80, 12535-44	4.2	8
100	The one-electron oxidation of a dithiolate molecule: the importance of chemical intuition. *Journal of Chemical Physics*, **2014**, 140, 18A519	3.9	8
99	Homolytic bond-dissociation enthalpies of tin bonds and tin ligand bond strengths A computational study. *Canadian Journal of Chemistry*, **2009**, 87, 974-983	0.9	8

98	Characterization of the bond between hydrogen and the non-nuclear attractor in anionic water clusters. *Physical Chemistry Chemical Physics*, **2008**, 10, 6814-9	3.6	8
97	Topological Analysis of Proteins as Derived from Medium and High-resolution Electron Density: Applications to Electrostatic Properties285-315		8
96	Atomic Response Properties61-94		8
95	A theoretical study of the fluorine valence shell in methyl fluoride. *Chemical Physics Letters*, **2005**, 403, 47-54	2.5	8
94	Cusp conditions for non-Coulombic interactions. *Computational and Theoretical Chemistry*, **2000**, 527, 27-33		8
93	Re-examination of the hyperfine structure of 14NH2. *Journal of Chemical Physics*, **1995**, 102, 3674-3678	3.9	8
92	Structure of PLi4 and Its Comparison with SiLi4, CLi4, and Li4: The Importance of Li-Li Interactions. *The Journal of Physical Chemistry*, **1995**, 99, 4941-4946		8
91	Equilibrium structures, proton affinities, and ionization potentials of the fluoroacetones. *Canadian Journal of Chemistry*, **1985**, 63, 836-842	0.9	8
90	The effect of protonic motion on the electronic properties of hydrogen-bonded complexes. *Computational and Theoretical Chemistry*, **1985**, 133, 45-58		8
89	The localized electrons detector as an ab initio representation of molecular structures. *International Journal of Quantum Chemistry*, **2010**, 110, n/a-n/a	2.1	7
88	Fundamentals in Tin Chemistry17-283		7
87	An Atoms in Molecules Study of the Halogen Resonance Effect. *Journal of Chemical Theory and Computation*, **2006**, 2, 271-80	6.4	7
86	Catalysis Mediated by Hydrogen Bonding: A Computational Study of the Aminolysis of 6-Chloropyrimidine. *Journal of the American Chemical Society*, **2000**, 122, 5384-5386	16.4	7
85	Hydrogen-bond mediated catalysis: the aminolysis of 6-chloropyrimidine as catalyzed by derivatives of uracil. *Journal of the American Chemical Society*, **2001**, 123, 2047-52	16.4	7
84	Electronic structures of the bound excited quartet states of the helium anion. *Physical Review A*, **1999**, 60, 4375-4378	2.6	7
83	Internal motion and the tunneling rates of CH+4 and CD+4. *Journal of Chemical Physics*, **1995**, 103, 8166-8173	3.9	7
82	The Electron Density as Calculated From Density Functional Theory. *Recent Advances in Computational*, **1995**, 369-401		7
81	Electronic structures and bonding in Rydberg molecules: NH4, H3O and related molecules. *Canadian Journal of Physics*, **1994**, 72, 851-855	1.1	7

80	Bond critical points in the electronic structures of binary hydrides. *International Journal of Quantum Chemistry*, **1986**, 29, 959-973	2.1	7
79	How does the geometry of the tetrahedral XF4−nCln (X = Al, Si, P) species depend on composition, or abinitiosicertumnescio. *Canadian Journal of Chemistry*, **1987**, 65, 1109-1123	0.9	7
78	Electronically excited states of chlorine monofluoride: A multi-reference configuration interaction study. *Chemical Physics*, **1988**, 121, 361-369	2.3	7
77	Molecular orbital structures of sulfones. *Canadian Journal of Chemistry*, **1982**, 60, 730-734	0.9	7
76	Theoretical study on the mechanism of iridium-catalyzed C–H functionalization of primary alkyl C–H bonds. *Canadian Journal of Chemistry*, **2016**, 94, 1028-1037	0.9	7
75	Interception of Nazarov Reactions of Allenyl Vinyl Ketones with Dienes: (3+2)- versus (4+3)-Cycloaddition and Subsequent Rearrangement. *European Journal of Organic Chemistry*, **2015**, 2015, 2952-2959	3.2	6
74	A computational investigation into the redox chemistry of Mo- and W-tris(diselenolene) complexes. *Structural Chemistry*, **2017**, 28, 1173-1180	1.8	6
73	Molecular docking study of macrocycles as Fk506-binding protein inhibitors. *Journal of Molecular Graphics and Modelling*, **2015**, 59, 117-22	2.8	6
72	Role of fluoride in accelerating the reactions of dialkylstannylene acetals. *Journal of Organic Chemistry*, **2015**, 80, 2989-3002	4.2	6
71	The convergence of basis set contractions: A case study of the molecular hyperfine structure of NH214. *Journal of Chemical Physics*, **1997**, 107, 6270-6274	3.9	6
70	Fragment Transferability Studied Theoretically and Experimentally with QTAIM Implications for Electron Density and Invariom Modeling317-341		6
69	Relationships between QTAIM and the Decomposition of the Interaction Energy Comparison of Different Kinds of Hydrogen Bond453-469		6
68	Ab initio and molecular dynamics study of dibenzotricyclic calcium antagonists: A rigid model approach. *International Journal of Quantum Chemistry*, **1994**, 52, 17-31	2.1	6
67	A 6-31G* chemistry of isoelectronic tetrahedral XL4 and YL4 (X = Li to F; Y = Na to Cl; L = H, F, Cl) species. Part 2. Energies, bond lengths, and critical radii. *Canadian Journal of Chemistry*, **1988**, 66, 2465-2475	0.9	6
66	Photochemical reactions of charge-transfer complexes. III. Molecular orbital studies of the charge-transfer complexes between 1,2-dimethoxyethylenes and 1,2-dicyanoethylenes. *Canadian Journal of Chemistry*, **1981**, 59, 974-981	0.9	6
65	Density Functional Theory Study of BF3-Mediated Additions of Enols and [(Trimethylsilyl)oxy]alkenes to an Oxyallyl Cation: Homologous Mukaiyama Reactions. *Journal of Physical Chemistry A*, **2015**, 119, 6714-22	2.8	5
64	Reaction of group 16 analogues of ethoxyquin with hydrogen peroxide: A computational study. *Computational and Theoretical Chemistry*, **2012**, 981, 68-72	2	5
63	Aromaticity Analysis by Means of the Quantum Theory of Atoms in Molecules399-423		5

62	The Lagrangian Approach to Chemistry35-59		5
61	HYDROXYL RADICAL REACTIONS IN BIOLOGICAL MEDIA. *Recent Advances in Computational*, **2002**, 387-415		5
60	Competing nitrile hydratase catalytic mechanisms: Is cysteine-sulfenic acid acting as a nucleophile?. *Computational and Theoretical Chemistry*, **2015**, 1070, 48-54	2	4
59	Computational insights into the suicide inhibition of Plasmodium falciparum Fk506-binding protein 35. *Bioorganic and Medicinal Chemistry Letters*, **2015**, 25, 3221-5	2.9	4
58	How do nucleophiles accelerate the reactions of dialkylstannylene acetals? The effects of adding fluoride to dialkoxydi-n-butylstannanes. *Journal of Physical Chemistry A*, **2013**, 117, 12648-57	2.8	4
57	Dramatic substituent effects on the mechanisms of nucleophilic attack on Se-S bridges. *Journal of Computational Chemistry*, **2013**, 34, 2537-47	3.5	4
56	Effect of counterions on the protonation state in a poly(G)-poly(C) radical cation. *Journal of Physical Chemistry B*, **2011**, 115, 14885-90	3.4	4
55	Radial moments of the electron density: Gas phase results and the effects of solvation. *Journal of Chemical Physics*, **2000**, 112, 1113-1121	3.9	4
54	Topological properties of the electronic structures of the reactants, transition states, and products of the reactions of the hydroxyl radical with the series C2HnF6□, n = 1□. *Canadian Journal of Chemistry*, **1996**, 74, 786-800	0.9	4
53	The relationship between the rate□quilibrium coefficient □ and transition state properties: a second-order M□ller□lesset perturbation study of SN2 reactions. *Canadian Journal of Chemistry*, **1992**, 70, 450-455	0.9	4
52	The effect of electron correlation on one-electron properties in the 2 3S and 2 1S excited states of the helium atom. *Chemical Physics Letters*, **1985**, 114, 197-200	2.5	4
51	The radius of the Fermi hole in atoms. *Journal of Physics B: Atomic and Molecular Physics*, **1985**, 18, L701-L705		4
50	One-proton and multiproton hydrogen bonds between ammonium ions and hydrogen fluoride. *Canadian Journal of Chemistry*, **1985**, 63, 1562-1567	0.9	4
49	Analysis of intramolecular hydrogen bonding in terms of the topological properties of the charge density. The protonated fluoroacetones. *Canadian Journal of Chemistry*, **1986**, 64, 2042-2047	0.9	4
48	Additivity model calculations of UHF spin densities and charge densities in methyl-substituted radical cations. *Theoretica Chimica Acta*, **1979**, 53, 309-317		4
47	Spin density distributions in some methyl substituted radical anions and cations. *Journal of the Chemical Society, Faraday Transactions 2*, **1979**, 75, 494		4
46	Chelotropic reactions: The thermal destruction of diazirine. *Tetrahedron Letters*, **1972**, 13, 4347-4350	2	4
45	Self-assembling ADADA helices formed by hydrogen bonding. *Journal of Physical Chemistry A*, **2012**, 116, 7965-75	2.8	3

44	Methods in Biocomputational Chemistry: A Lesson from the Amino Acids **2010**, 403-421		3
43	An orbital-based density difference index for the comparison of electron density distributions. *Journal of Chemical Physics*, **1997**, 107, 6693-6698	3.9	3
42	Fleshing-out Pharmacophores with Volume Rendering of the Laplacian of the Charge Density and Hyperwall Visualization Technology499-514		3
41	The ELF Topological Analysis Contribution to Conceptual Chemistry and Phenomenological Models141-162		3
40	Atoms in Molecules Theory for Exploring the Nature of the Active Sites on Surfaces231-256		3
39	A Non-Born□Oppenheimer Self-consistent Field Method. *Journal of Mathematical Chemistry*, **2007**, 42, 353-365	2.1	3
38	Theoretical study of the thermolysis of beta-hydroxyl aldehydes. *Journal of Physical Chemistry A*, **2006**, 110, 8710-8	2.8	3
37	The host□guest inclusion complex of p-chlorophenol inside □-cyclodextrin: An atoms in molecules study. *Chemical Physics Letters*, **2005**, 416, 70-74	2.5	3
36	A multi-component model for radiation damage to DNA from its constituents. *Theoretical and Computational Chemistry*, **2001**, 9, 409-466		3
35	A spin-density polarization index. *Journal of Chemical Physics*, **1998**, 108, 2824-2830	3.9	3
34	Mechanism of C2H4 dehydrogenation to C2H2 on the Ni(111) surface. *Chemical Physics Letters*, **1996**, 253, 129-134	2.5	3
33	Multiplicities of □ylide ground states: Computational evidence for a breakdown of aromaticity arguments. *Journal of Physical Organic Chemistry*, **1991**, 4, 566-572	2.1	3
32	Topological evidence for an N?N bond in cis-1,2-dinitrosoethene: The remarkable structure of the di-N-oxide of 1,2-diazacyclobutadiene. *Journal of Physical Organic Chemistry*, **1990**, 3, 143-146	2.1	3
31	The Importance of the MM Environment and the Selection of the QM Method in QM/MM Calculations: Applications to Enzymatic Reactions. *Advances in Protein Chemistry and Structural Biology*, **2015**, 100, 153-85	5.3	2
30	The catalytic formation of leukotriene C4: a critical step in inflammatory processes. *Physical Chemistry Chemical Physics*, **2014**, 16, 16284-9	3.6	2
29	A theoretical study of the structure and conductivity of polycytosineacetylene. *Chemical Physics Letters*, **2011**, 506, 243-247	2.5	2
28	Interactions Involving Metals □From □hemical Categories□to QTAIM, and Backwards343-374		2
27	Applications of the Quantum Theory of Atoms in Molecules in Organic Chemistry □Charge Distribution, Conformational Analysis and Molecular Interactions375-397		2

26	Solid State Applications of QTAIM and the Source Function Molecular Crystals, Surfaces, HostGuest Systems and Molecular Complexes163-206		2
25	Modeling the reaction mechanisms for redox regulation of protein tyrosine phosphatase 1B activity. *Theoretical Chemistry Accounts*, **2007**, 118, 573-578	1.9	2
24	The Development of Computational Chemistry in Canada. *Reviews in Computational Chemistry*, **2007**, 213-299		2
23	Preparation and evaluation of novel stationary phases for improved chromatographic purification of pneumocandin B0. *Journal of Chromatography A*, **2006**, 1101, 204-13	4.5	2
22	On the choice of the active space and the basis set for MCSCF calculations on small molecules and reactive surfaces. *The Journal of Physical Chemistry*, **1993**, 97, 11969-11973		2
21	The acidity of phosphoglucomutase monofluoromethylenephosphonate ligands probed by NMR spectroscopy and quantum mechanical methods. *Canadian Journal of Chemistry*, **2016**, 94, 902-908	0.9	2
20	Lewis Acid-Mediated Cyclization of Allenyl Aryl Ketones. *Journal of Organic Chemistry*, **2019**, 84, 13665-13675	4.7	1
19	The Calculation of the Hyperfine Coupling Tensors of Biological Radicals. *Progress in Theoretical Chemistry and Physics*, **2013**, 285-322	0.6	1
18	Stabilizing effect of solvent and guest residue amino acids on a model alpha-helix peptide. *Computational and Theoretical Chemistry*, **2012**, 998, 80-86	2	1
17	Reply to the Comment on 'Theoretical Study of Polaron Formation in Poly(G)Poly(C) Cations' *Journal of Physical Chemistry B*, **2011**, 115, 8949-8950	3.4	1
16	Topology and Properties of the Electron Density in Solids207-229		1
15	Calibration of a computational scheme for solvation studies: halide ions bound to water X(H2O) (X = F, Cl, Br). *Molecular Physics*, **2006**, 104, 389-394	1.7	1
14	ELECTRON CORRELATION STUDIES BY MEANS OF ELECTRON-PAIR DENSITY FUNCTIONS **2002**, 577-611		1
13	Density difference representation of the charge clouds of the monatomic ions of the alkali halides. *Journal of Molecular Structure*, **1983**, 92, 167-171	3.4	1
12	On the possibility of isolating diazirine N-oxides. *Journal of Heterocyclic Chemistry*, **1983**, 20, 767-768	1.9	1
11	Trans -stilbene in methanol solution. *Molecular Physics*, **1995**, 86, 327-346	1.7	1
10	QTAIM Analysis of Raman Scattering Intensities: Insights into the Relationship Between Molecular Structure and Electronic Charge Flow95-120		0
9	Richard (Rick) Francis Langler Memorial Issue. *Australian Journal of Chemistry*, **2015**, 68, 349	1.2	

8	Quantum Mechanical Approaches to Selenium Biochemistry **2010**, 585-603	
7	A simple representation of energy matrix elements in terms of symmetry-invariant bases. *Journal of Computational Chemistry*, **2010**, 31, 492-6	3.5
6	Computation of Hyperfine Coupling Tensors to Complement EPR Experiments **2004**, 565-580	
5	Trans-stilbene in methanol solution On the effect of flexible atomic charges in computer simulations. *Molecular Physics*, **1995**, 86, 327-346	1.7
4	Density difference representation of the charge clouds of the monatomic ions of the alkali halides. *Computational and Theoretical Chemistry*, **1983**, 92, 167-171	
3	Spin density distributions in radical anions of heterocyclic amine N-oxides. *Theoretica Chimica Acta*, **1980**, 57, 163-168	
2	Electron correlation, isoelectronic, isonuclear, spin, and excitation aspects of Politzer–Parr partitioning. *Journal of Chemical Physics*, **1980**, 72, 5399-5404	3.9
1	The Calculation of the Hyperfine Coupling Tensors of Biological Radicals. *Progress in Theoretical Chemistry and Physics*, **2003**, 239-265	0.6